NASA TECHNICAL MEMORANDUM

NASA TM X-52060

NASA TM X-52060

N64-32436
(ACCESSION NUMBER)
5
(PAGES)
TMX-52060
(NASA CR OR TMX OR AD NUMBER)
(THRU)
1
(CODE)
11
(CATEGORY)
FACILITY FORM 602

# CESIUM-CESIUM CROSS SECTION AND THE LENNARD-JONES PARAMETERS

OTS PRICE

XEROX $ 1.00 PH

MICROFILM $ .50 MF

by John W. Sheldon
Lewis Research Center
Cleveland, Ohio

TECHNICAL PREPRINT prepared for Thermionic Conversion Specialist Conference sponsored by the Institute of Electrical and Electronics Engineers
Cleveland, Ohio, October 26-28, 1964

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION · WASHINGTON, D.C. · 1964

# CESIUM-CESIUM CROSS SECTION AND THE LENNARD-JONES PARAMETERS

by John W. Sheldon
Lewis Research Center
Cleveland, Ohio

TECHNICAL PREPRINT prepared for

Thermionic Conversion Specialist Conference sponsored by
the Institute of Electrical and Electronics Engineers
Cleveland, Ohio, October 26-28, 1964

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

# CESIUM-CESIUM CROSS SECTION AND

# THE LENNARD-JONES PARAMETERS

by John W. Sheldon

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio

E-2753

32436

Abstract

The values of the Lennard-Jones parameters used by Robinson (Advanced Energy Conversion, 3, 19 (1963)) in his computation of the transport properties of cesium vapor are used to compute the cesium-cesium total scattering cross section. The result gives good agreement with beam experiments. Author

---

It is well known that the diameter of an atom may be estimated from the solid density. The corresponding hand-sphere atomic cross section may be used to estimate gas thermal conductivity, viscosity, and diffusion coefficient[1]. Such estimates have been made for cesium by several workers[2,3]. A more rigorous procedure has been detailed by Hirschfelder, et al[4]. The differential scattering cross section obtained from an appropriate interaction potential is used to compute the transport cross section. The values of the parameters in the interaction potential are obtained from the atomic structure. Robinson[5] has used a Lennard-Jones (12-6) potential to compute the transport properties of a cesium vapor by this procedure and achieved reasonable agreement with experiment[6].

The application of hard-sphere theory to the highly polarizable cesium atom is certainly open to question. The usual justification for the hard-sphere approach is that reliable values of the parameters in the Lennard-Jones potential are not available. The purpose of this note is to lend credence to theoretical Lennard-Jones parameters for cesium-cesium interactions.

TM X-52060

The Lennard-Jones interaction potential $V(r)$ is given[4] by

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad (1)$$

where the parameter $\sigma$ is the separation, r, at which the inverse $12^{th}$ repulsive potential is just balanced by the inverse $6^{th}$ attractive potential. The dispersion parameter, $\epsilon$, gives the depth of the potential well.

Since the scattering of thermal atomic beams is dominated by the attractive portion of this potential[7], then

$$V(r) \simeq - 4\epsilon\left(\frac{\sigma}{r}\right)^{6} \qquad (2)$$

Using this potential in the Massey-Mohr approximation[7] yields the following value for Q, the total scattering cross section:

$$Q(v) = \frac{9\pi}{4}\left(\frac{3\pi}{2}\frac{\epsilon\sigma^6}{\hbar v}\right)^{2/5} \qquad (3)$$

where $\hbar$ is Planck's constant divided by $2\pi$ and v is the relative velocity of the colliding atoms.

The dispersion energy constant, $4\epsilon\sigma^6$, has been computed by Fontana[9] to be $2.2\times10^{-57}$ erg-cm$^6$ for a cesium-cesium interaction. Following Rothe and Bernstein's[10] outline for the application of Slater and Kirkwood's[11] procedure, $3.43\times10^{-57}$ erg-cm$^6$ is obtained for the dispersion energy constant. Using a mean value of $2.81\times10^{-57}$ erg-cm$^6$ in equation (3) yields

$$Q(v) = \frac{1.45\times10^{5}}{v^{2/5}} \text{ Å}^2 \qquad (4)$$

where v is given in cm/sec.

When an atomic cesium beam emitted from an oven at $450^{\circ}$ K is scattered by cesium vapor at about $340^{\circ}$ K, the mean relative velocity of the particles is approximately $3.7\times10^4$ cm/sec (using the method of ref. 10 to estimate the relative velocity). Equation (4) then gives

$$Q(3.7\times10^4 \text{ cm/sec}) = 2150 \text{ Å}^2$$

Estermann, et al[12] experimentally obtained a value of 2350 $\text{Å}^2$ for these temperatures.

## REFERENCES


1. R. D. Present: Kinetic Theory of Gases. McGraw-Hill Book Co., Inc. (1958).
2. W. R. Martini, Advanced Energy Conversion 3, 49 (1963).
3. M. Gottlieb and R. J. Zollweg, Advanced Energy Conversion 3, 37 (1963).
4. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird: Molecular Theory of Gases and Liquids. John Wiley & Sons, Inc. (1954).
5. L. B. Robinson, Advanced Energy Conversion 3, 19 (1963).
6. S. Kitrilakis and M. Meeker, Advanced Energy Conversion 3, 59 (1963).
7. R. B. Bernstein, Jour. Chem. Phys. 34, 361 (1961).
8. H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. A144, 188 (1934).
9. P. R. Fontana, Phys. Rev. 123, 1865 (1961).
10. E. W. Rothe and R. B. Bernstein, Jour. Chem. Phys. 31, 1619 (1959).
11. J. C. Slater and J. G. Kirkwood, Phys. Rev. 37, 682 (1931).
12. I. Estermann, S. N. Foner and O. Stern, Phys. Rev. 71, 250 (1947).